

Message

From: Washington, John [Washington.John@epa.gov]
Sent: 12/5/2017 1:46:13 PM
To: Lindstrom, Andrew [Lindstrom.Andrew@epa.gov]; Strynar, Mark [Strynar.Mark@epa.gov]; McCord, James [mccord.james@epa.gov]; Buckley, Timothy [Buckley.Timothy@epa.gov]
Subject: RE: spectra and initial observations

Hi Andy,

Your attachment helped. The description of the hexafluoropropylidene sounds consistent with the spectrum – at least at the level of the general description (see image below from page 13). The spectra I sent looks as though it could be similar to hexafluoropropylidene units alternating with CH₂ units.

Among things that call for attention, though, is why the spectrum seems dominated by m/z values consistent with CF₃ and H bound to chains related to C₈ length in particular (i.e., there was the C₈, the C₁₆ = 2xC₈ and the C₇ which looked as though a terminal CH₂ might have been cleaved from C₈). But there were not other prominent repeating spectral increments. When I first saw the spectrum, I was expecting to solve for m/z values consistent with a wide range of chain lengths so the spectrum might have been fragments of a 3D polymeric lattice.

Maybe a possible cause for specific chain lengths is I notice on the Saint Gobain site that its performance plastics page lists two films, Chemfilm and Norfilm. Maybe films are chain-length specific? Here is the site:

<https://saint-gobain-northamerica.com/business/product-categories/performance-plastics>

John

Image below from page 13:

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treatments of leather, textile and other substrate, cladding for optical fibers, etc. (Drobny, 2001).

4.4.2 Hexafluoroisopropylidene-containing polymers

Monomers containing the hexafluoroisopropylidene (6F) group have found worldwide application in the synthesis of high-performance polymers. These polymers show dramatic improvement of properties when compared to non-fluorinated analogues. In general the presence of the 6F group in a polymer increases solubility, oxidative and thermal stability, optical transparency, flame resistance and resistance to UV mediated degradation, while decreases crystallinity, dielectric constant, water absorption and surface energy.

Numerous applications for polymers containing hexafluoroisopropylidene groups have been suggested, including water and heat resistant coatings, fibers, adhesives and even dental prostheses. The high cost of these materials, however, limits their use to small-scale and speciality applications such as microelectronics, aerospace and medical devices (Scheirs, 1997).

From: Lindstrom, Andrew
Sent: Tuesday, December 05, 2017 6:37 AM
To: Washington, John <Washington.John@epa.gov>; Strynar, Mark <Strynar.Mark@epa.gov>; McCord, James

<mccord.james@epa.gov>; Buckley, Timothy <Buckley.Timothy@epa.gov>

Subject: RE: spectra and initial observations

John,

Do you have any idea what temperature the stack is operating at?

I've attached a Norwegian report on incineration of PFAS which could be helpful in describing what may be produced here.

Thank you,

Andy

From: Washington, John

Sent: Monday, December 4, 2017 5:24 PM

To: Strynar, Mark <Strynar.Mark@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>; McCord, James <mccord.james@epa.gov>; Buckley, Timothy <Buckley.Timothy@epa.gov>

Subject: spectra and initial observations

OK I took a break from sieving NJ soils and trying to fix the tandem MS to summarize a little on this spectrum.

First though, my Waters instruments are not on the lab LAN or internet → endless computer rules.

I am attaching the spectra, initial observations, thoughts, calculated masses agreeing with the spectra, and example structure for one of the masses.

On my regular ramp, this peak comes off at 0.72 minutes, not far from solvent surge. I tried starting the ramp way down at 95% water, 5% ACN and the peak still came off at about the same time, maybe as late as 0.78 minutes.

On the attached file, I just noticed two colors look similar. On the original, and for my intent, each of the 3 peak series are supposed to be different colors to help guide my intended message.

At this early stage, it look like maybe a series of C8 masses, a series of C16 masses and a series of C7 masses. The C7 masses look as though maybe a CH2 was cleaved from a C8 mass.

John